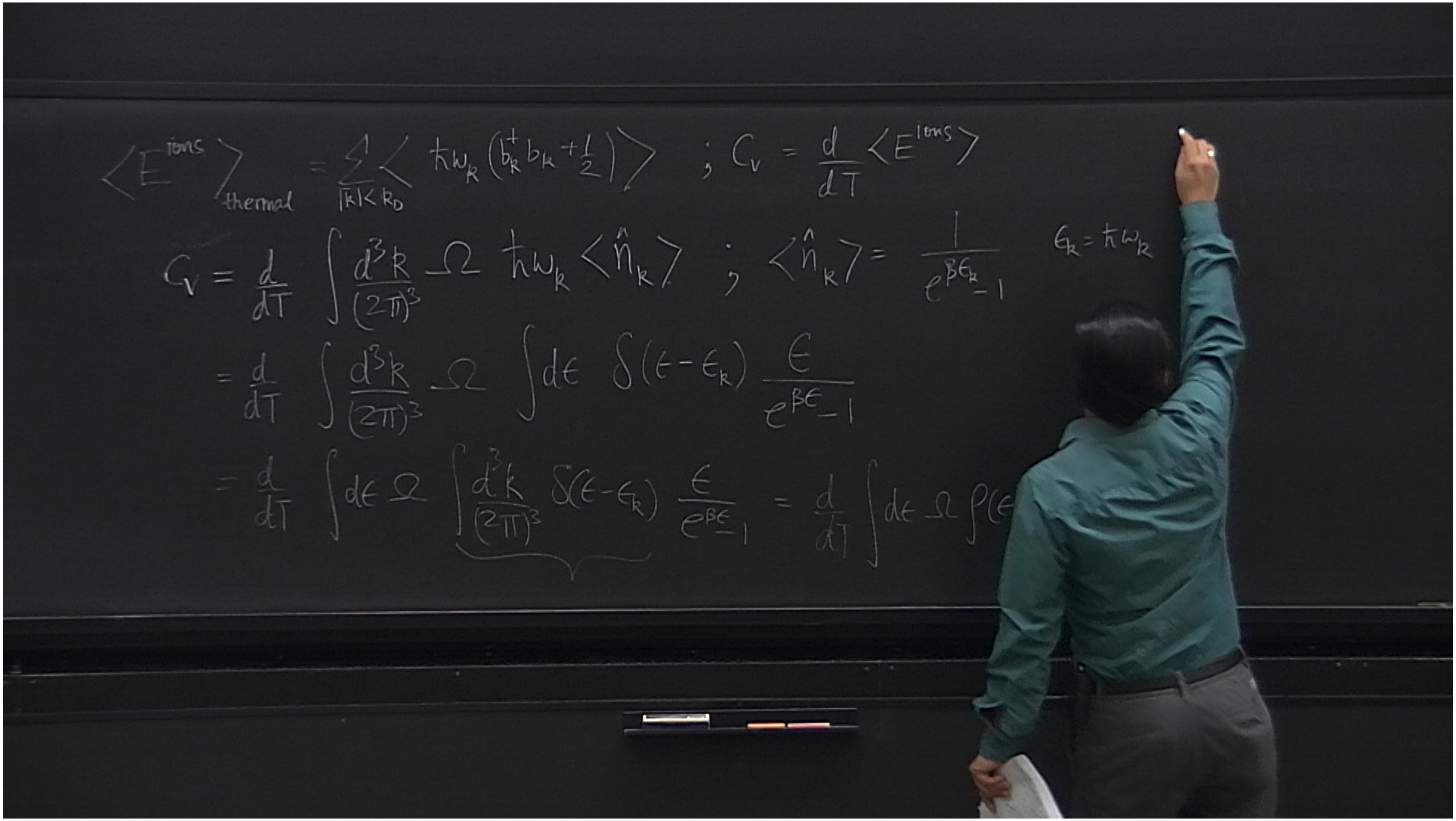
Title: PSI 17/18 - Condensed Matter - Lecture 8

Date: Nov 15, 2017 10:45 AM

URL: http://pirsa.org/17110033

Abstract:



$\langle E^{ions}\rangle_{thermal} = \sum_{|k|<k_D} \langle \hbar\omega_k (b_k^\dagger b_k + \frac{1}{2})\rangle$; $C_v = \frac{d}{dT}\langle E^{ions}\rangle$
$C_v = \frac{d}{dT}\int \frac{d^3k}{(2\pi)^3}\,\Omega\,\hbar\omega_k\langle\hat{n}_k\rangle$; $\langle \hat{n}_k\rangle = \frac{1}{e^{\beta\epsilon_k}-1}$
$\epsilon_k = \hbar\omega_k$
$= \frac{d}{dT}\int\frac{d^3k}{(2\pi)^3}\,\Omega\int d\epsilon\,\delta(\epsilon-\epsilon_k)\frac{\epsilon}{e^{\beta\epsilon}-1}$
$= \frac{d}{dT}\int d\epsilon\,\Omega \underbrace{\int\frac{d^3k}{(2\pi)^3}\delta(\epsilon-\epsilon_k)}\frac{\epsilon}{e^{\beta\epsilon}-1} = \frac{d}{dT}\int d\epsilon\,\Omega\,\rho(\epsilon$

Electron phonon interaction

$$\hat{V}_{ion-el} = \sum_{i,n} V(|r_i - R_n|) \quad r_i \equiv \text{electronic position operator}$$
$$R_n \equiv \text{ionic} \quad ''$$

$$= \sum_{i,n} \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{|r_i - R_n|}$$

$$V(r_i, R_n) |\psi_m, \psi_n\rangle = \sum_{jk} V^{mn}_{jk} |\psi_j, \psi_k\rangle$$

$$V^{mn}_{jk} = \langle \psi_j, \psi_k | V(r_i R_n) | \psi_m \psi_n \rangle$$

$$\hat{V}_{tot} = \sum_{m,n,jk} V^{mn}_{jk} b^+_j b^+_k b_m b_n$$

$$\bar{R}_n = \bar{R}_n^{\,0} + \bar{u}_n$$

$$\hat{V}_{ion\text{-}el} = \underbrace{\sum_{i,n} V(\bar{r}_i - \bar{R}_n^{\,0})}_{\text{Bloch bands}} - \underbrace{\sum_{i,n} \bar{u}_n \cdot \nabla_{\bar{R}_n} V(\bar{r}_i - R_n)\Big|_{\bar{R}_n = \bar{R}_n^{\,0}}}_{\text{electron phonon interactions}}$$

$$\hat{T}_{tot} = \sum_{j,k} T_{jk}\, b_j^{\dagger} b_k = \sum_{\bar{k}} \frac{\hbar^2 |\bar{k}|^2}{2m}\, c_{\bar{k}}^{\dagger} c_{\bar{k}}$$

$$H_{el-ph} = -\sum_{\substack{n \\ k'\sigma' \\ k\sigma}} \bar{u}_n \cdot \langle k'\sigma' | \nabla_{\bar{R}_n} V(\bar{r}-\bar{R}_n)\Big|_{\bar{R}_n=\bar{R}_n^0} | k\sigma \rangle \, c^{+}_{k'\sigma'} c_{k\sigma}$$

$$= -\sum_{n} \bar{u}_n \cdot \sum_{\substack{kk' \\ \sigma}} \int d^3\bar{r} \; \varphi^{*}_{k'}(\bar{r}) \, \nabla_{\bar{R}_n} V(\bar{r}-\bar{R}_n)\Big|_{\bar{R}_n=\bar{R}_n^0} \varphi_{k}(\bar{r}) \, c^{+}_{k'\sigma} c_{k\sigma}$$

$$H_{el\text{-}ph} = -\sum_{\substack{n \\ k'\sigma' \\ k\sigma}} \bar{u}_n \cdot \langle k'\sigma' | \nabla_{\bar{R}_n} V(\bar{r}-\bar{R}_n)\big|_{\bar{R}_n=\bar{R}_n^0} | k\sigma \rangle \, c^{\dagger}_{k'\sigma'} c_{k\sigma}$$

$$= -\sum_{n} \bar{u}_n \cdot \sum_{\substack{k k' \\ \sigma}} \int d^3 \bar{r} \; \varphi^{*}_{k'}(\bar{r}) \, \nabla_{\bar{R}_n} V(\bar{r}-\bar{R}_n)\big|_{\bar{R}_n=\bar{R}_n^0} \, \varphi_k(\bar{r}) \, c^{\dagger}_{k'\sigma} c_{k\sigma}$$

$$H_{el-ph} = -\sum_{\substack{n \\ k'\sigma' \\ k\sigma}} \bar{u}_n \cdot \langle k'\sigma' | \nabla_{\bar{R}_n} V(\bar{r} - \bar{R}_n)\big|_{\bar{R}_n = \bar{R}_n^0} | k\sigma \rangle \, c^\dagger_{k'\sigma'} c_{k\sigma}$$

$$= -\sum_n \bar{u}_n \cdot \sum_{\substack{k k' \\ \sigma}} \int d^3 r \; \varphi^*_{k'}(\bar{r}) \, \nabla_{\bar{R}_n} V(\bar{r} - \bar{R}_n)\big|_{\bar{R}_n = \bar{R}_n^0} \, \varphi_k(\bar{r}) \, c^\dagger_{k'\sigma} c_{k\sigma}$$

$$\varphi_{\bar{k}}(\bar{r} + \bar{R}_n^0) = e^{i \bar{k} \cdot \bar{R}_n^0} \varphi_{\bar{k}}(\bar{r})$$

$$\left\langle k' \right| \nabla_{\bar{R}_n} V(|\bar{r}-\bar{R}_n|)\Big|_{\bar{R}_n=\bar{R}_n^0} \left| k \right\rangle$$

$\uparrow$ Replace $\bar{r} = \bar{r} - \bar{R}_n^0$

$$= e^{i(\bar{k}-\bar{k}')\cdot\bar{R}_n^0} \int d^3(\bar{r}-\bar{R}_n^0)\; \varphi^*_{\bar{k}'}(\bar{r}-\bar{R}_n^0)\; \nabla_{\bar{R}_n} V(\bar{r}-\bar{R}_n)\Big|_{\bar{R}_n=\bar{R}_n^0}\; \varphi_{\bar{k}}(\bar{r}-\bar{R}_n^0)$$

$$= e^{i(\bar{k}-\bar{k}')\cdot\bar{R}_n^0}\; S_{\bar{k}\bar{k}'}$$

$$H_{el\text{-}ph} = -\sum_{kk'\sigma} S_{kk'} \cdot \sum_n e^{i(\bar{k}-\bar{k}')\cdot R_n^0}\, \bar{u}_n\, c^\dagger_{k'\sigma} c_{k\sigma}$$

$$\Big|_{\bar{R}_n=\bar{R}_n^0} \varphi_{\bar{k}}(\bar{r}-\bar{R}_n^0)$$

$$^{+}_{k\sigma} c_{k\sigma}$$

$$u_n = \frac{1}{\sqrt{N}} \sum_k e^{ikan} Q_k \quad \text{and} \quad Q_k = \sqrt{\frac{\hbar}{2M\omega_k}} \left(b^{+}_{-k} + b_k \right)$$

$$\bar{u}_n = \frac{1}{\sqrt{N}} \sum_{\substack{q\lambda \\ q \in FBZ}} \sqrt{\frac{\hbar}{2M\omega_\lambda(q)}} \, e^{i\bar{q}\cdot\bar{R}_n^0} \left(b^{+}_{-q,\lambda} + b_{q,\lambda} \right) \bar{A}_\lambda$$

$\lambda \in$ All phonon branches

$$u_n = \frac{1}{\sqrt{N}} \sum_k e^{ikan} Q_k \quad \text{and} \quad Q_k = \sqrt{\frac{\hbar}{2M\omega_k}} \left(b^{+}_{-k} + b_k \right)$$

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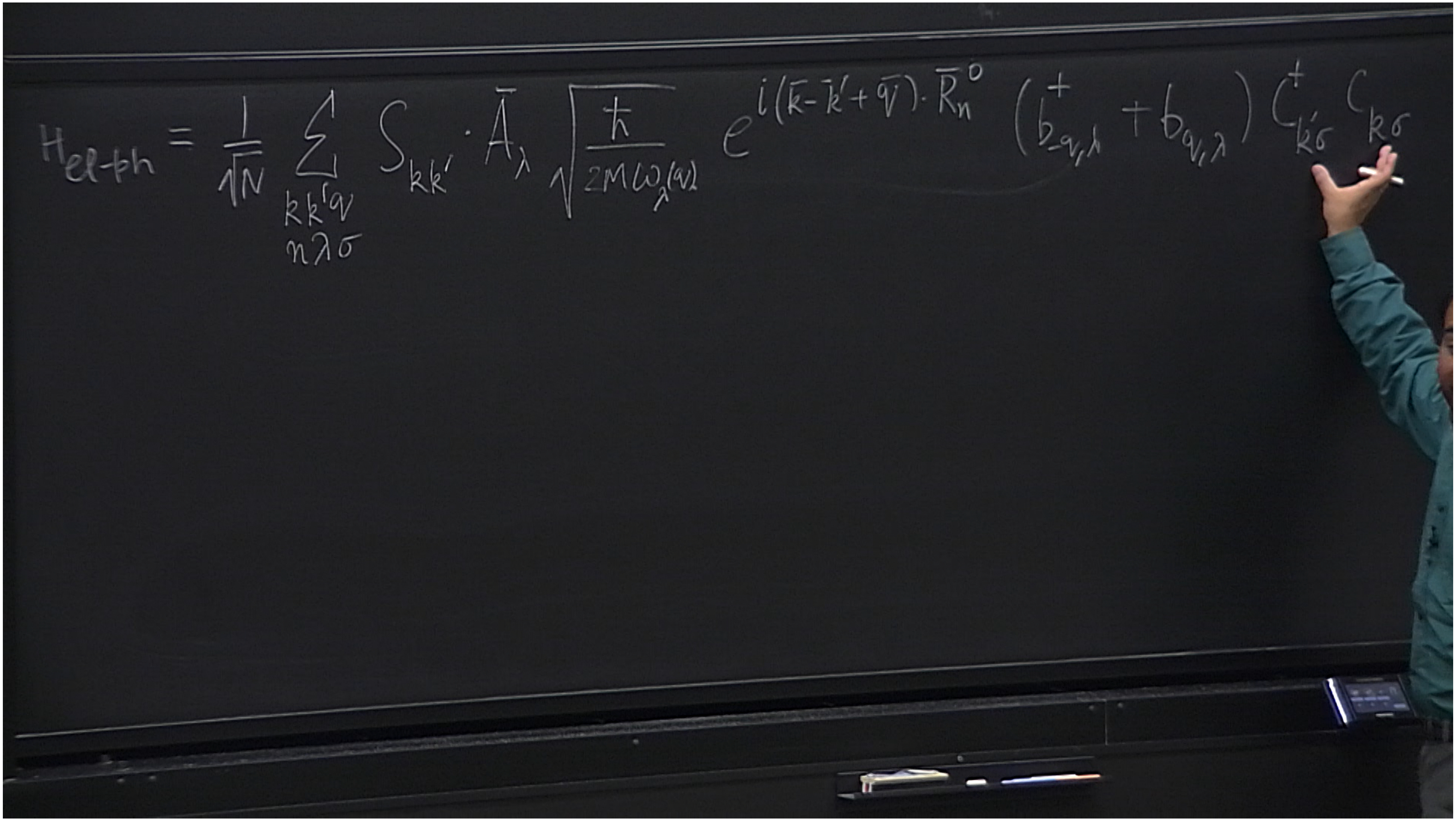
$\lambda \in$ All phonon branches

$\bar{A}_\lambda \equiv$ polarization for the λ^{th} branch

$$\sum_G \delta_{\bar{k}-\bar{k}', -\bar{G}}$$

$$= \sum_G \frac{1}{N} \sum_n e^{i(\bar{k}-\bar{k}'+\bar{G})\bar{R}_n^0}$$

$$= \frac{1}{N} \sum_{\bar{G}} \sum_{\bar{n}} e^{i(\bar{k}-\bar{k}')\cdot\bar{R}_n^0}$$

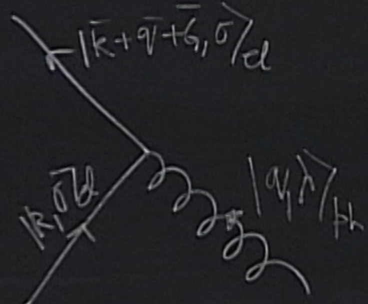

$$H_{el\text{-}ph} = \frac{1}{\sqrt{N}} \sum_{\substack{kk'q \\ n\lambda\sigma}} S_{kk'} \cdot \bar{A}_\lambda \sqrt{\frac{\hbar}{2M\omega_\lambda(q)}}\, e^{i(\bar{k}-\bar{k}'+\bar{q})\cdot\bar{R}_n^0} \left(b^\dagger_{-q,\lambda} + b_{q,\lambda}\right) c^\dagger_{k'\sigma} c_{k\sigma}$$

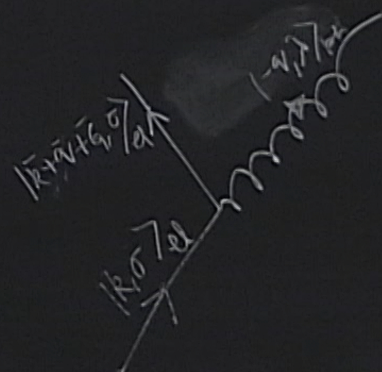
$$= \frac{1}{\sqrt{N}} \sum_{\substack{k k' q \\ n \lambda \sigma}} S_{kk'} \cdot \bar{A}_\lambda \sqrt{\frac{\hbar}{2M\omega_\lambda(q)}}\, e^{i(\bar{k}-\bar{k}'+\bar{q})\cdot \bar{R}_n^0} \left(b^\dagger_{-q,\lambda} + b_{q,\lambda} \right) c^\dagger_{k'\sigma} c_{k\sigma}$$

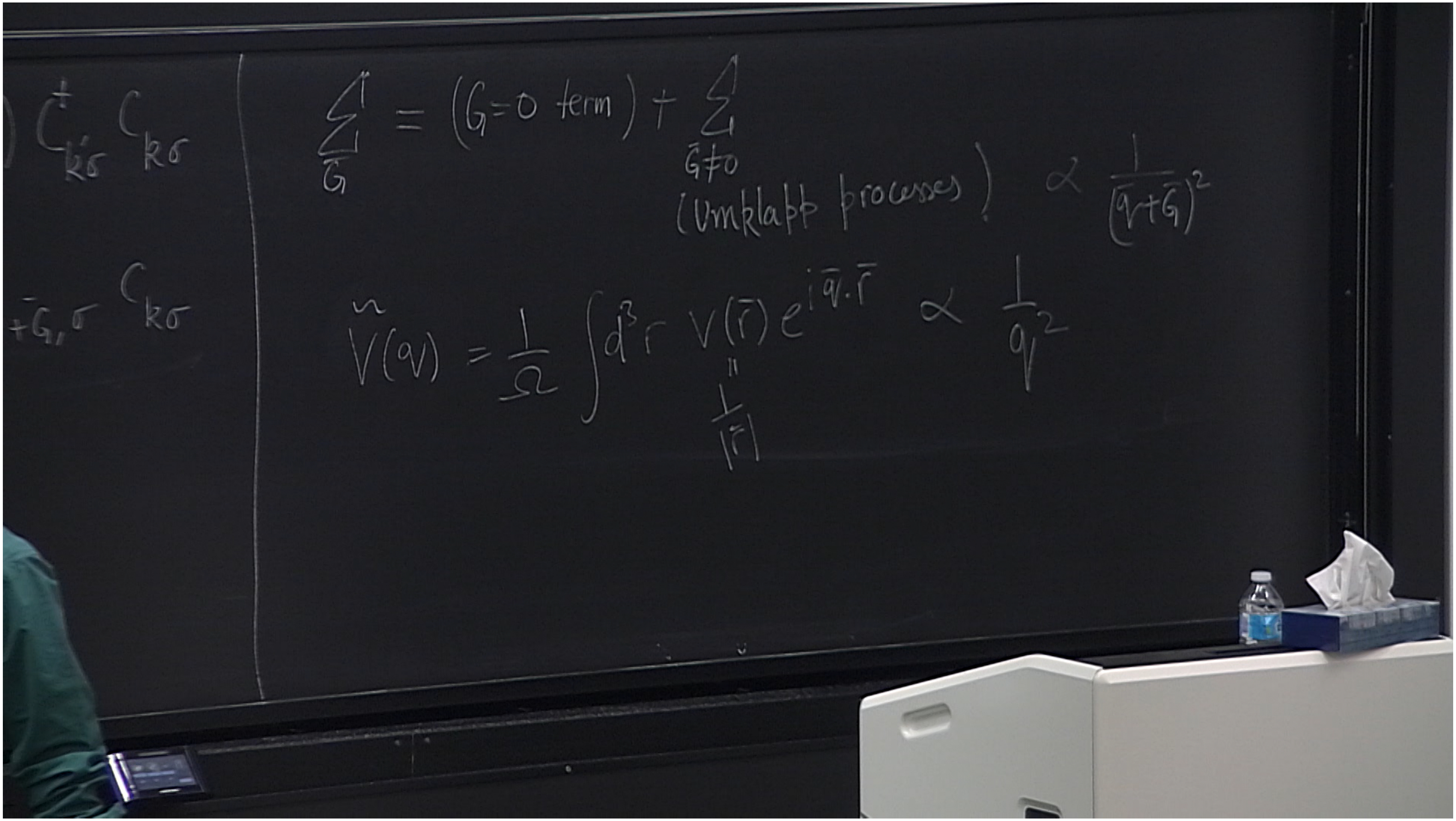
$$= \frac{1}{\sqrt{N}} \sum_{\substack{k q \bar{G} \\ \lambda \sigma}} S_{\bar{k},\bar{k}+\bar{q}+\bar{G}} \cdot \bar{A}_\lambda \sqrt{\frac{\hbar}{2M\omega_\lambda(q)}} \left(b^\dagger_{-q,\lambda} + b_{q,\lambda} \right) c^\dagger_{\bar{k}+\bar{q}+\bar{G},\sigma} c_{k\sigma}$$

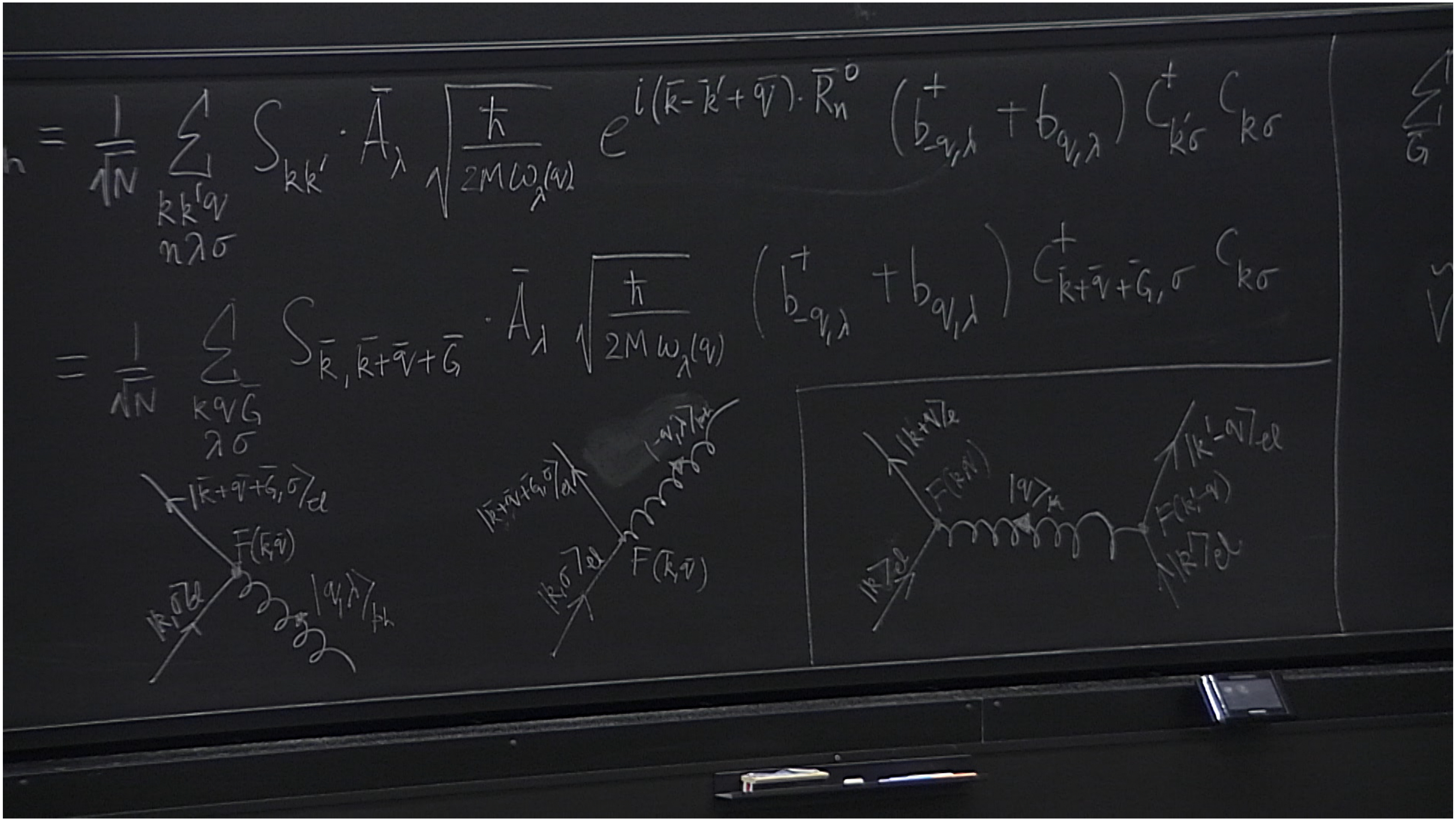
$$H_{el\text{-}ph} = \frac{1}{\sqrt{N}} \sum_{\substack{k k' q \\ n \lambda \sigma}} S_{kk'} \cdot \bar{A}_\lambda \sqrt{\frac{\hbar}{2M\omega_\lambda(q)}}\, e^{i(\bar{k}-\bar{k}'+\bar{q})\cdot \bar{R}_n^0} \left(b^\dagger_{-q,\lambda} + b_{q,\lambda}\right) c^\dagger_{k'\sigma} c_{k\sigma}$$

$$= \frac{1}{\sqrt{N}} \sum_{\substack{k q \bar{G} \\ \lambda \sigma}} S_{\bar{k},\bar{k}+\bar{q}+\bar{G}} \cdot \bar{A}_\lambda \sqrt{\frac{\hbar}{2M\omega_\lambda(q)}} \left(b^\dagger_{-q,\lambda} + b_{q,\lambda}\right) c^\dagger_{\bar{k}+\bar{q}+\bar{G},\sigma} c_{k\sigma}$$






$C^{\dagger}_{k'\sigma} \; C_{k\sigma}$
$_{+\bar{G},\sigma} \; C_{k\sigma}$
$\sum_{\bar{G}} = (G=0 \text{ term}) + \sum_{\bar{G}\neq 0}$
(Umklapp processes) $\propto \frac{1}{(\bar{q}+\bar{G})^2}$
$\tilde{V}(q) = \frac{1}{\Omega} \int d^3r \, V(\bar{r}) \, e^{i\bar{q}\cdot\bar{r}} \propto \frac{1}{q^2}$
$V(\bar{r}) = \frac{1}{|\bar{r}|}$



$= \frac{1}{\sqrt{N}} \sum_{k k' q n \lambda \sigma} S_{kk'} \cdot \bar{A}_\lambda \sqrt{\frac{\hbar}{2M\omega_\lambda(q)}} e^{i(\bar{k}-\bar{k}'+\bar{q})\cdot \bar{R}_n^0} (b^\dagger_{-q,\lambda} + b_{q,\lambda}) C^\dagger_{k'\sigma} C_{k\sigma}$
$= \frac{1}{\sqrt{N}} \sum_{k q G \lambda \sigma} S_{\bar{k}, \bar{k}+\bar{q}+\bar{G}} \cdot \bar{A}_\lambda \sqrt{\frac{\hbar}{2M\omega_\lambda(q)}} (b^\dagger_{-q,\lambda} + b_{q,\lambda}) C^\dagger_{\bar{k}+\bar{q}+\bar{G},\sigma} C_{k\sigma}$
$|\bar{k}+\bar{q}+\bar{G},\sigma\rangle_{el}$
$F(\bar{k},\bar{q})$
$|k,\sigma\rangle_{el}$
$|q,\lambda\rangle_{ph}$
$|\bar{k}+\bar{q}+\bar{G},\sigma\rangle_{el}$
$|-q,\lambda\rangle_{ph}$
$|k,\sigma\rangle_{el}$
$F(\bar{k},\bar{q})$
$|k+q\rangle_{el}$
$F(k,q)$
$|q\rangle_{ph}$
$|k\rangle_{el}$
$|k'-q\rangle_{el}$
$F(k',-q)$
$|k'\rangle_{el}$

$c_{k\sigma} c_{k\sigma}$

Schrieffer-Wolff transformation

$$U = e^{S}, \quad U^\dagger = e^{S^\dagger} = e^{-S} \qquad \boxed{S^\dagger = -S}$$

$$\tilde{H} = U^\dagger H U = e^{-S} H e^{S} = H - [S,H] + \frac{(-1)^2}{2}[S,[S,H]] + (\dots)$$

$c^\dagger_{k\sigma} c_{k\sigma}$

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$$\hat{H} = U^\dagger H U = e^{-S} H e^{S} = H - [S,H] + \frac{(-1)^2}{2}[S,[S,H]] + (\dots)$$

$H = H_0 + H_{el\text{-}ph}$ where $H_0 = H_{el} + H_{ph}$

$$[S, H_0] = H_{el\text{-}ph}$$

$$\hat{H} = H_0 - [S, H_{el\text{-}ph}] + \frac{1}{2}[S, H_{el\text{-}ph}] + \frac{1}{2}[S,[S,H_{el\text{-}ph}]] + (\dots)$$

$c_{k\sigma} c_{k\sigma}$

Schrieffer-Wolff transformation

$$U = e^{S}, \quad U^{\dagger} = e^{S^{\dagger}} = e^{-S} \qquad \boxed{S^{\dagger} = -S}$$

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$H = H_0 + H_{el\text{-}ph}$ where $H_0 = H_{el} + H_{ph}$

$$[S,H_0] = H_{el\text{-}ph}$$

$$\tilde{H} = H_0 - [S,H_{el\text{-}ph}] + \frac{1}{2}[S,H_{el\text{-}ph}] + \overbrace{\frac{1}{2}[S,[S,H_{el\text{-}ph}]]}^{O(F^3)} + (\dots)$$

$$\ddot{H} = H_0 - \frac{1}{2}\left[S, H_{el-ph}\right] + O(P^3 \text{ or higher})$$

$$S = \sum_{\bar{k},\bar{q}} F(k,q)\, C^{+}_{\bar{k}+\bar{q}} C_{\bar{k}} \left(y\, b^{+}_{-\bar{q}} + x\, b_{\bar{q}} \right)$$

Using this Ansatz & demanding $[S, H_0] = H_{el-ph}$

$$x = \frac{1}{\epsilon_{\bar{k}+\bar{q}} - \epsilon_{\bar{k}} - \hbar\omega(q)} \quad \text{and} \quad y = \frac{1}{\epsilon_{\bar{k}+\bar{q}} - \epsilon_{\bar{k}} + \hbar\omega(q)}$$

$$\tilde{H} = H_0 - \frac{1}{2}\left[S, H_{el-ph}\right] + O(F^3 \text{ or higher})$$

$$S = \sum_{\bar{k},\bar{q}} F(k,q)\, c^\dagger_{\bar{k}+\bar{q}}\, c_{\bar{k}} \left(y\, b^\dagger_{-\bar{q}} + x\, b_{\bar{q}} \right)$$

Using this Ansatz & demanding $[S, H_0] = H_{el-ph}$

$$x = \frac{1}{\epsilon_{\bar{k}+\bar{q}} - \epsilon_{\bar{k}} - \hbar\omega(q)} \quad \text{and} \quad y = \frac{1}{\epsilon_{\bar{k}+\bar{q}} - \epsilon_{\bar{k}} + \hbar\omega(q)}$$

$$-\frac{1}{2}\left[S, H_{el-ph}\right]$$

$$\boxed{\left[b_{q}, b^{\dagger}_{-q}\right] = \delta_{q,-q}}$$

$$\hat{H} = H_{el} + H_{ph} + \sum_{k k' q} \frac{F(k,q)\,F(k'-q)\,\hbar\omega(q)}{\left(\epsilon_{k+q} - \epsilon_{k}\right)^{2} - \left(\hbar\omega(q)\right)^{2}}\, c^{\dagger}_{k+q}\, c^{\dagger}_{k'-q}\, c_{k'}\, c_{k}$$

el-ph

$\omega(q)$

$$-\frac{1}{2}\left[S, H_{el-ph}\right]$$

$$\tilde{H} = H_{el} + H_{ph} + \sum_{k k' q} \frac{F(k,q)\,F(k'-q)\,\left(\hbar\omega(q)\right)}{\left(\epsilon_{k+q}-\epsilon_{k}\right)^2-\left(\hbar\omega(q)\right)^2}\, c^\dagger_{k+q}\, c^\dagger_{k'-q}\, c_{k'}\, c_{k}$$

$$\boxed{\left[b_{q},\, b^\dagger_{-q'}\right] = \delta_{q,-q'}}$$

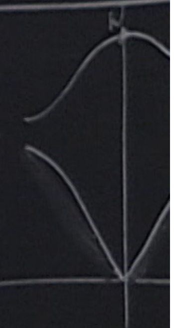
H_{el-ph}

$\hbar\omega(q)$

Consider $q \to 0$, $\omega(q) = \text{Constant} \neq 0$ for optical phonons

Consider TWO electrons close to the Fermi Sea

$$\left(\epsilon_{k+q}-\epsilon_{k}\right)^2 = \frac{\hbar^2 (k_F+q)^2}{2m} - \frac{\hbar^2 k_F^2}{2m} \longrightarrow 0 \text{ as } q \to 0$$



$$\frac{1}{2}[S, H_{el-ph}]$$

$$\hat{H} = H_{el} + H_{ph} + \sum_{k k' q} \frac{F(k,q)\,F(k',-q)\,\hbar\omega(q)}{(\epsilon_{\bar{k}+\bar{q}} - \epsilon_{\bar{k}})^2 - (\hbar\omega(q))^2}\, c^\dagger_{\bar{k}+\bar{q}}\, c^\dagger_{\bar{k}'-\bar{q}}\, c_{\bar{k}'}\, c_{\bar{k}}$$

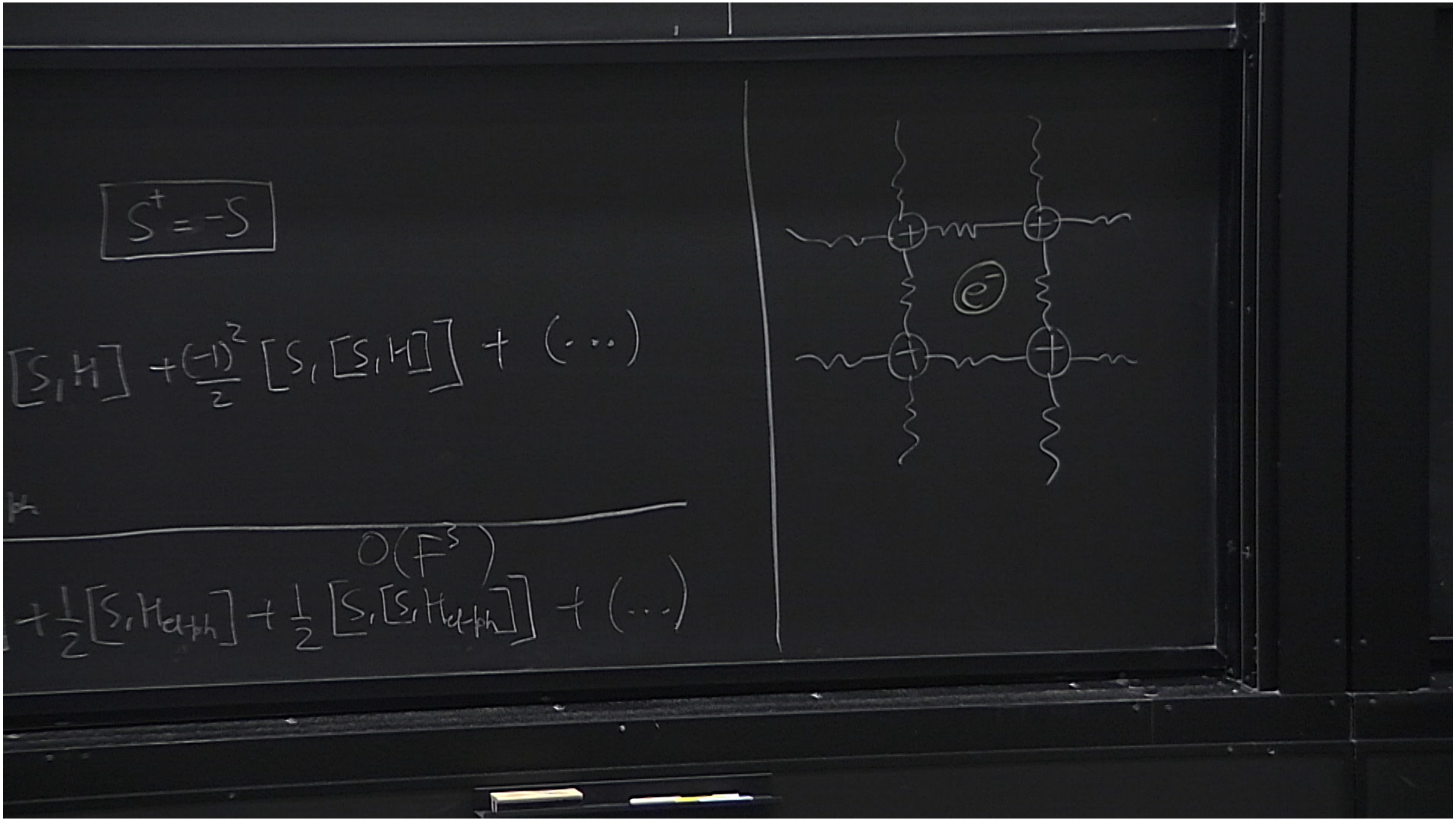
$$\boxed{[b_q, b^\dagger_{-q}] = \delta_{q,-q}}$$

Consider $q \to 0$, $\omega(q) =$ Constant $\neq 0$ for optical phonons

Consider TWO electrons close to the Fermi Sea

$$(\epsilon_{k+q} - \epsilon_k)^2 = \frac{\hbar^2 (k_F+q)^2}{2m} - \frac{\hbar^2 k_F^2}{2m} \longrightarrow 0 \text{ as } q \to 0$$

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$


$S^{\dagger} = -S$
$[S,H] + \frac{(-1)^2}{2}[S,[S,H]] + (\dots)$
$O(F^3)$
$+ \frac{1}{2}[S,H_{el-ph}] + \frac{1}{2}[S,[S,H_{el-ph}]] + (\dots)$
e^-